

Hexyl acetate
142-92-7 | DTXSID6022006

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.89e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.12e-01

Confidence level: 6.81e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Hexyl acetate</div> <div>Measured: 3.54e-03</div> <div>Predicted: 6.89e-03</div>	<div>Image not found</div> <div>Ethyl hexanoate</div> <div>Measured: 4.36e-03</div> <div>Predicted: 6.07e-03</div>	<div>Image not found</div> <div>1,3-Dimethylbutyl acetate</div> <div>Measured: 9.01e-03</div> <div>Predicted: 8.99e-03</div>
<div>Image not found</div> <div>Acetic acid, 2-ethylbutyl ester</div> <div>Measured: 4.44e-02</div> <div>Predicted: 1.03e-02</div>	<div>Image not found</div> <div>Pentyl propionate</div> <div>Measured: 5.62e-03</div> <div>Predicted: 7.41e-03</div>	